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Physical Studies, Inc.
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PROTON AND ELECTRON SCATTERING BY DIATOMIC MOLECULES

by

R. G. BREENE, Jr.

1 April 1963

Final Report

Contract Number AF19(628)-476

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Project 8658
Task 86580

Prepared For

AIR FORCE CAMBRIDGE RESEARCH LABORATORIES
OFFICE OF AEROSPACE RESEARCH
UNITED STATES AIR FORCE
BEDFORD, MASSACHUSETTS

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INTRODUCTION

The first, short section gives a brief introduction to the scattering matrix. In the next two sections we consider the heart of our present problem. Section II deals with the scattering of electrons by diatomic molecules, specifically oxygen. The treatment is restricted in such a way that electronic computing machinery is not requisite to the final solution. In the electron case the Born approximation is, of course, applicable and we carry the problem to the point where a numerical solution, which could readily be carried out on a desk calculator, is required. In Section III the proton-molecule scattering problem is discussed, specifically proton scattering by oxygen. The Born approximation is not applicable in this case. We begin by carrying a distorted wave treatment to the point where a very small set of one dimensional differential equations are obtained. The equations are not solved although their hand solution would pose no particular problem. We then consider the impact parameter treatment of this same proton-oxygen problem. For the familiar two-state case we carry through the problem to obtain the total cross-sections. In addition, we introduce a general multi-state treatment of this impact parameter problem which is not specifically applied. In both these latter sections target distortion by the projectile particle is included in the scattering potential. The last section is concerned with additions to Professor Takayanagi's bibliography.

SECTION I

THE SCATTERING MATRIX*

We consider first the scattering of electrons by diatomic molecules in the energy range from one to fifty thousand electron volts. One here encounters elastic, inelastic, and charge exchange scattering where the inelastic scattering may involve electronic, vibrational, and rotational excitation, ionization, and dissociation either alone or in combination. As an example of what may occur we remark the following reactions :

$AB + e = AB + e$	(elastic)
$AB + e = AB + e$	(charge exchange)
$AB + e = AB^* + e$	(inelastic)
$AB + e = AB^+ + 2e$	(ionization)
$AB + e = A + B + e$	(dissociation)

which may of course also occur in any combination.

In considering the problem we may begin by indicating the scattering matrix form although the individual elements therein will not be evaluated until a later stage in the development. The wave function for the electron in the absence of the neutral molecule will have the asymptotic form

$$\varphi_\gamma(r) \sim v_\gamma^{-\frac{1}{2}} r^{-1} A_\gamma \left[\exp\left\{-i\left(k_\gamma r - l\tfrac{\pi}{2}\right)\right\} - \exp\left\{+i\left(k_\gamma r - l\tfrac{\pi}{2}\right)\right\} \right] \qquad (1)$$

*The material in this section is of a review nature. References are provided in Section IV and in the Takayanagi review.

in the case where the electron is in channel γ. The normalization is to unit amplitude at infinity. The first term in the bracket represents the incoming electron while the second term represents the outgoing. We shall define the term "channel" after our introduction of the scatterer. When we introduce the scatterer we have the following expression for the free electron in the presence of the molecule:

$$\varphi_\gamma(r) \sim v_\gamma^{-1/2} r^{-1} \left[A_\gamma \exp\{-i(k_\gamma r - l\tfrac{\pi}{2})\} - B_\gamma \exp\{i(k_\gamma r - l\tfrac{\pi}{2})\} \right] \qquad (2)$$

We now define "channel" as a specific set of parameters defining the translational state of the electron and the electronic-vibration-rotation state of the molecule. In an elastic collision the electron-molecule system will re-enter the entry channel after collision. We now consider the exit channel parameter, B_γ, for the case of an elastic collision.

In order to do so we consider the familiar asymptotic solution for the l-th partial wave for a potential falling off more rapidly than r^{-2}.

$$\frac{1}{kr} \sin(kr - l\tfrac{\pi}{2} + \delta_l) \qquad (3)$$

This may be re-written as

$$\frac{1}{2ikr} \left[e^{i\delta_l} e^{i(kr - l\frac{\pi}{2})} - e^{-i\delta_l} e^{-i(kr - l\frac{\pi}{2})} \right]$$

$$= -\frac{e^{-i\delta_l}}{2ikr} \left[e^{-i(kr - l\frac{\pi}{2})} - S_l e^{i(kr - l\frac{\pi}{2})} \right] \qquad (4)$$

where we now define the factor S_ℓ as the scattering matrix element. It is apparent that it gives us the ratio of the outgoing to the incoming waves thus yielding at least one description of the scattering. In terms of the channel dispersion parameters, A_γ and B_γ, this may be written:

$$S_\ell = \frac{B_\gamma}{A_\gamma} \tag{5}$$

Now we remark that in our elastic case above the exit channel parameter was of amplitude equal to that of the entrance channel parameter. This, of course, would not be the case in inelastic scattering. In that situation the system sometimes departs partially through the entrance channel. However it departs partially through at least one additional channel so that entry and exit amplitudes must differ. Here again, however, the matrix element is still defined by the channel parameter ratios. The diagonal elements correspond to the ratios between the elastic paraments (A_γ and B_γ). The inelastically scattered electron has only an outgoing wave viz:

$$\Phi_{\gamma'}(r) \sim v_\gamma^{-1/2} r^{-1} B_{\gamma'} \exp[i(k_{\gamma'} r - \ell\pi)] \tag{6}$$

The off-diagonal elements in the scattering matrix then are given by the ratio $B_{\gamma'}/A_\gamma$. We discuss the scattering matrix no further but refer the reader to the extensive work which has been done in this field in recent years.

In introducing the scattering matrix we have in Eq. (1) assumed the partial wave form for the free electron. The reader will, of course,

recall that the partial wave is specified by the momentum quantum number "ℓ" in the above equations. Although the partial wave analysis is used quite extensively in actual scattering problems, we revert to a more general form in what follows:

SECTION II

ELECTRON SCATTERING BY DIATOMICS*

A. General Formulation of the Problem

First, we are going to assume that the Franck-Condon principle is operative, that is, we suppose that the molecular wave function can be written as a product of electronic, vibrational, and rotational wave functions. Therefore we are going to somewhat simplify the following by considering only the electronic function, the vibrational and rotational being possible of later consideration.

The wave function for the molecule - electron system is taken as:

$$\Psi = \sum_{ie} P_{ie} \Phi_{An}(\underline{r}_i) \chi^{+}(\underline{r}_e) \psi_{n^+}(\underline{r}) + \sum_{ie} P_{ie} \Phi_{An}(\underline{r}_i) \chi^{-}(\underline{r}_e) \psi_{n^-}(\underline{r}) \quad (7)$$

In Eq. (6) P_{ie} is the permutation operator; $\Phi_{An}(\underline{r}_i)$ is the molecular wave function and consists of a simple product of the molecular orbitals. We have, of course, assumed a single determinant LCAO-MO form for the molecular wave function.

We take H_{mol} to be the Hamiltonian for the molecule in the absence of any external interaction. The interaction Hamiltonian will be

$$H_{int} = -\frac{Z_a}{r_{ae}} - \frac{Z_b}{r_{be}} + \sum_{i=1}^{Z_a+Z_b} \frac{1}{r_{ie}} \quad (8a)$$

*The general development general case and Born approximation are discussed in Theory of Atomic Collisions, Quantum Theory I. Elements etc.

which leads to:

$$\left(H_{mol} - \tfrac{1}{2}\nabla_e^2 - \frac{k_n^2}{2} - \frac{Z_a}{r_{ae}} - \frac{Z_b}{r_{be}} + \sum \frac{1}{r_{ie}} - E_n\right)\Psi = 0 \tag{8b}$$

Under the constraint

$$(H_{mol} - E_n)\,\Phi_{An}(\underline{r}_i) = 0$$

and after substitution for Ψ Eq (8b) becomes:

$$\left[\nabla_e^2 + k_n^2 + 2\left(\frac{Z_a}{r_{ae}} + \frac{Z_b}{r_{be}} - \sum \frac{1}{r_{ie}}\right)\right]\left[\sum_{ie} P\,\Phi_{An}(\underline{r}_i)\,\chi^+(\underline{r}_e)\,\psi_n(\underline{r})\right.$$

$$\left. + \sum_{ie} P\,\Phi_{An}(\underline{r}_i)\,\chi^-(\underline{r}_e)\,\psi_n(\underline{r})\right] = 0 \tag{9}$$

The $\chi_n^{\pm}$ are spin functions for the free electron, χ_n^+ referring to a free electron spin parallel to the molecular spin, χ_n^- referring to the anti-parallel situation. Now multiply through on the left by the plus spin function and integrate appropriately to get

$$\sum_{ie} P\,\Phi_{An}(\underline{r}_i)\left[\nabla_e^2 + k_n^2 + 2\left(\frac{Z_a}{r_{ae}} + \frac{Z_b}{r_{be}} - \sum \frac{1}{r_{ie}}\right)\right]\psi_n(\underline{r}) = 0 \tag{10}$$

Further we now suppose that the molecule is stationary so that $\underline{r}$ becomes $\underline{r}_e$, the coordinate of the free electron referred to the center-of-mass of the molecule as a coordinate center. Next the specific product nature of Φ_{An} is introduced.

$$\bar{\Phi}_{An}(\underline{r}_i) = \frac{1}{\sqrt{Z_a + Z_b}} \prod_{\alpha} \varphi_{n\alpha}$$

and we multiply Eq. (10) through on the left by $\bar{\Phi}_{An}$ and integrate over all space. The result is:

$$\{\nabla_j^2 + k_n^2 - U_{nn}\}\psi_{ne}(j) - \sum_{\alpha} \int K_{nn}(\underline{r}_i, \underline{r}_j)\psi_{n\alpha}(i)\, d\tau_i$$

$$= \sum_{m \neq n} \{U_{nm}\psi_{me}(j) + \sum_{\alpha} \int K_{nm}(\underline{r}_i, \underline{r}_j)\psi_{m\alpha}(i)\, d\tau_i\} \quad (11a)$$

$$U_{nm} = -\frac{1}{Z_a + Z_b} \sum_{\alpha} \int \varphi_{n\alpha}^*(i)\varphi_{m\alpha}(i) \sum H_{ij}\, d\tau_i \quad (11b)$$

$$\sum_{\alpha} \int K_{nm}(\underline{r}_i, \underline{r}_j)\psi_{m\alpha}(i)\, d\tau_i = \sum_{\alpha} \frac{1}{Z_a + Z_b} \int \varphi_{m\alpha}(j)\varphi_{n\alpha}^*(i)\{H_i - \sum H_{ij}\}\psi_{m\alpha}(i)\, d\tau_i \quad (11c)$$

where

$$H_j = \nabla_j^2 + k_m^2 \quad (12a)$$

$$H_{ij} = 2\left(\frac{Z_a}{r_{aj}} + \frac{Z_b}{r_{bj}} - \sum \frac{1}{r_{ij}}\right) \quad (12b)$$

Now note that in Eq. (11c) the individual molecular orbitals must have their spins parallel to that of the free electron. Finally, one is able to apply Green's Theorem to Eq. (11c) with the result:

$$\sum_{\alpha} \int K_{nm}(\underline{r}_i, \underline{r}_j)\psi_{m\alpha}(i)\, d\tau_i = \frac{1}{Z_a + Z_b} \sum_{\alpha} \int \varphi_{m\alpha}(j)\varphi_{m\alpha}(i)\{k_m^2 - 2(E_{n\alpha} + \sum \tfrac{1}{r_{ij}})\}\varphi_{n\alpha}^*(i)\, d\tau_i \quad (11c')$$

Eqs. (11a),)11b), and (11c') are the general forms for the free elec-

tron wave function where spin-orbit type interactions have been left out of the original Hamiltonian. These rather fine interactions appear to have no particular place in this treatment. Some simplification of these equations has to be made in order to carry their solution any further. A number of such approximations have been made most of them having to do with the relative magnitude of the U_{nm} and K_{nm}.

The most drastic assumptions lead to the Born approximation where, in effect, one supposes that the scattering molecule is hardly there at all. We shall show that this appears adequate for the molecule-electron scattering and inadequate for the molecule-proton scattering case.

B. The Born Approximation for Electron Excitation

As we remarked above, the Born approximation is basically predicated on a rather small interaction between electron and molecule. Under these conditions, we suppose the diagonal elements in Eqs. (11) to be zero, and we replace ψ on the right hand side of the equation by the plane wave:

$$\exp(ik\underline{n}\cdot\underline{r})$$

If we now eliminate exchange from the equation; the result is:

$$\{\nabla_j^2 + k_n^2\}\psi_{ne}(j) = U_{nm}\exp(ik_m\underline{n}_m\cdot\underline{r}_j) \tag{13a}$$

On the other hand if the exchange term is maintained we obtain:

$$\{\nabla_j^2 + k_n^2\}\psi_{ne}(j) = U_{nm}\exp(ik_m\underline{n}_m\cdot\underline{r}_j) + \frac{1}{Z_a+Z_b}\sum_a\int\{\phi_{na}(j)\phi^*_{n\alpha}(i)\{k_n^2$$

$$-2(E_{na}+\sum\frac{1}{r_{ij}})\}\exp(ik_m\underline{n}_m\cdot\underline{r}_i)d\tau_i \tag{13b}$$

We consider Eq. (13a). It is well known that the solution to the equation,

$$\nabla^2\psi + k^2\psi = F(\underline{r})$$

is:

$$\psi = G(\underline{r}) - \frac{1}{4\pi}\int \frac{\exp(ik|\underline{r}-\underline{r}'|)}{|\underline{r}-\underline{r}'|} F(\underline{r}')\,d\tau'$$

where:

$$\nabla^2 G + k^2 G = 0$$

In quite precise analogy we may write the solution to Eq. (13a) as

$$\psi_{ne} = \exp(ik_n \underline{n}_n \cdot \underline{r}_j) - \frac{1}{4\pi}\int \frac{\exp(ik_n|\underline{r}_j - \underline{r}'|)}{|\underline{r}_j - \underline{r}'|} \cdot U_{nm}(\underline{r}') \exp(ik_m \underline{n}_m \cdot \underline{r}')\,d\tau' \qquad (14)$$

We may now use this expression to obtain the scattering cross section for the general case. It should be remarked here that the source of difficulty in Eq. (14) is, of course going to be U_{nm} to which we return shortly. For now, however, we recall that the cross section makes use of the scattering amplitude which in turn is available from the asymptotic form of the wave function. The asymptotic form of Eq. (14) is:

$$\psi_{ne} \sim \frac{1}{4\pi r} e^{ik_n r}\int \exp\{i(k_m \underline{n}_m - k_n \underline{n}_n)\cdot \underline{r}_j\} U_{nm}(\underline{r}')\,d\tau' \qquad (15)$$

from which we obtain the cross section for scattering of the system into the n-th channel, the electron undergoing a deflection through an angle ϑ :

$$\sigma_n(\vartheta) = \frac{k_n}{k_m}\frac{1}{4\pi^2}\left|\int \exp\{i(k_m \underline{n}_m - k_n \underline{n}_n)\cdot \underline{r}_j\} U_{nm}(\underline{r}')\,d\tau'\right|^2 d\tau \qquad (16)$$

Eq. (16) is written in atomic units, and k_n refers to the entry channel. In essence the collision has induced a transition from molecular state "m" to molecular state "n" and a change of free electron linear momentum from k_m to k_n. Eq. (16) is, of course the required result. Before considering it in more detail we inquire of its validity.

The requirement which must be fulfilled in this electron - molecule case is: the velocity of the free electron must be much larger than the velocity of the orbital electrons. If we suppose something like one-half of the orbital energy is associated with kinetic energy of the orbital electrons then we may compare this energy to the translational energy of the incident electron.

The $2\sigma_g$, $2\sigma_u$ and $3\sigma_g$ electrons in oxygen, for example, have kinetic energies of around ten or twenty electron volts. Thus, one thousand volt electrons should be sufficiently energetic. We therefore accept the Born approximation for this problem and return our attention to what we may designate "the potential", namely U_{nm}.

We are using a simple determinant LCAO-MO form for the molecular wave function. Let us suppose that:

(1) The state "n" differs from the state "m" in only one orbital and

(2) The orbitals that remain the same are orthonormal and the orbital which changes is orthogonal to the one which does not.

Actually we can check with little difficulty on the two electron-jump case at some later point. We shall consider Eq. (11b) later; we now write

the diagonal element as:

$$\frac{2(Z_a+Z_b-1)}{(Z_a+Z_b)}\left[\frac{Z_a}{r_{ij}}+\frac{Z_b}{r_{ij}}\right]-2\sum_{\alpha}\sum_{j}\int\frac{|\varphi_{n\alpha}^{*}(\underline{r}_i)|^2}{r_{ij}}d\underline{r}_i=U_{nn} \qquad (17)$$

We consider Eq. (17). If for the $\varphi_{n\alpha}$ we take the un-perturbed molecular orbital, Eq. (17) will yield, in essence, the Coulomb potential produced by the isolated molecule. It has been shown recently[1], in the case of two oxygen molecules that this potential is particularly unrealistic. In order to get the proper repulsive form for the potential it was necessary to introduce the reciprocal effect of the other molecule on this potential. The Coulomb potential alone yielded a nice attractive potential. Therefore, there does not appear to be any point in taking the $\varphi_{n\alpha}$ as unperturbed orbitals. On the other hand we do not wish to go back beyond the Born beginning to the coupled set through which polarization can be introduced automatically. Therefore we may sensibly begin with molecular orbitals already distorted by the presence of the free electron. This we have done recently in the case of molecule-molecule collisions.[1]

On the other hand we might take the type potential used by Fisk[2] in his treatment of the scattering of slow electrons. If "d" is the internuclear separation in the molecule and "r_1", and "r_2" the free electron separation from the two nuclei then the following coordinates may be adopted:

$$\xi=\frac{r_1+r_2}{d} \qquad \eta=\frac{r_1-r_2}{d}$$

Then the potential due to the nuclei may be written:

$$\Phi_c = 2Z\left(\frac{1}{r_1} + \frac{1}{r_2}\right) = \frac{8Z}{d}\frac{\xi}{\xi^2-\eta^2} \tag{18}$$

In order for this to approximately represent the field of the molecule, it must go to zero at some boundary, say, $\xi = \xi_0$ = constant. Fisk selects functions f (ξ) to multiply Φ_c and produce a potential function which meets the following criteria

$$f(1) = 1 \quad , \quad f'(\xi_0) \leq 0$$
$$f(\xi_0) = 0 \quad , \quad f'(1) \leq 0 \tag{19}$$

Of several forms for f (ξ) considered Fisk settled on:

$$f(\xi) = 1 - [\xi_0/(\xi_0-1)^2][(\xi-1)^2/\xi] \tag{20}$$

Stier[3] had previously appealed to the following form for this function

$$f(\xi) = [(\xi_0 - \xi)/(\xi_0 - 1)]^2$$

At any rate a value for ξ_0 is chosen, and, after the evaluation of the integral over the charge density, a factor is determined to correct the atomic number in Eq. (18). This essentially completes Fisk's evaluation of his potential. He then proceeds to evaluate the elastic scattering cross section for a number of molecules including oxygen and nitrogen. This evaluation itself is, of course, available and could be extended to the energies of our interest. On the one hand it has the advantage over the Born

approximation of yielding precise results for the scattering while on the other hand it has the disadvantage which arises from the approximate nature of its potential.

We could develop a Coulomb potential for the isolated molecule which would be quite general. However, it becomes somewhat more complicated when the polarization of the molecular charge cloud by the free electron is included. In this case one must first obtain expressions for the molecular orbitals distorted by the free electron. This can, of course, be accomplished for the general case on a digital computer. Since we do not intend to appeal to computing machinery at this stage we restrict the position of the free electron to either the internuclear axis of the molecule or the plane perpendicular to this axis and containing the center-of-mass of the molecule. For the present we shall restrict ourselves to the latter path.

In arriving at our potential we first determine the form for the perturbed MO's. We begin with the on-axis case. The form for the distorted molecular orbital is as follows:[1,4]

$$\chi_i = [1 + a_i r_i \cos\theta_i]\,\chi_i^{(0)} \tag{21a}$$

where $\chi_i^{(0)}$ is the undistorted molecular orbital and "a_i" is a parameter. The angle θ_i is referred to the center-of-mass of the molecule. The parameter a_i is given by:

$$a_i = \frac{(\chi_j^{(0)}|H'|\chi_i^{(0)})}{(\chi_j^{(0)}|\cos\vartheta_i|\chi_i^{(0)})(E_i^\circ - E_j^\circ)} \tag{21b}$$

where:

$$H' = -\frac{1}{R} + \frac{1}{r} \tag{21c}$$

The matrix elements of $\cos\vartheta_i$ have already been evaluated.[4] The evaluation of the matrix elements of H' remain to be carried out. Having obtained this distortion we shall now apply it to each of the two atomic orbitals in the molecule. This will yield the potential in which our free electron exists. This potential in turn is to be used in Eq. (16) to obtain the scattering cross section.

In evaluating these matrix elements we first specifically restrict ourselves to oxygen. Next we note the MO's whose distortion we consider;[5]

$$2\sigma_g = .5641\sigma_g 2s + .1677\sigma_g 2p \tag{22a}$$

$$3\sigma_g = -.3117\sigma_g 2s + .6148\sigma_g 2p \tag{22b}$$

$$2\sigma_u = .7500\sigma_u 2s - .1617\sigma_u 2p \tag{22c}$$

$$3\sigma_u = .5345\sigma_u 2s + .9275\sigma_u 2p \tag{22d}$$

The matrix elements between pairs of these orbitals will then consist of obvious linear combinations of matrix elements over the orbitals $\sigma_g 2s$ and $\sigma_g 2p$. We remark that there can be no difference between such gerade

and ungerade matrix elements. The reason for this may be explained as follows.

In the on-axis case one can readily demonstrate that the contribution to the matrix element from the nether nucleus is negligible. This means in essence:

$$\sigma_\delta 2s = A(e^{-\delta r_a} + e^{-\delta r_b}) = Ae^{-\delta r_b}, \text{ etc.}$$

so that our integrals simplify considerably. We shall follow through the evaluation of the first of these matrix elements. The general expression will be:

$$(\sigma_g 2s|H'|\sigma_g 2s) = \frac{\delta^5}{3\pi}\iiint \frac{r^2 e^{-2\delta r}}{r_{ij}} r^2 \sin\nu \, dr\,d\nu\,d\varphi - \frac{1}{R} \qquad (23)$$

wherein the r_{ij} represents the separation of the electron from the element of the molecular charge cloud under consideration. The "r" represents the MO coordinate referred to the nucleus closest to the perturbing proton. The effective nuclear charge has a value of 2.275. The familiar Legendre expansion reduces as follows for this case:

$$\frac{1}{r_{ij}} = \sum \frac{(k-|m|)!}{(k+|m|)!} \frac{r_<^k}{r_>^{k+1}} P_k^{|m|}(\cos\nu) \exp\left[im(\varphi-\Phi)\right] = \sum \frac{r_<^k}{r_>^{k+1}} P_k^0(\cos\nu) \qquad (24)$$

For the $\sigma_g 2s$ case all terms in Eq. (24) save the first (k = 0) will disappear during angular integration so that there results:

$$(\sigma_g 2s|H'|\sigma_g 2s) = \frac{4}{3}\delta^5\left\{e^{-2\delta R}\left[\frac{R}{(2\delta)^2} + \frac{6R}{(2\delta)^3} + \frac{18}{(2\delta)^4} + \frac{24}{(2\delta)^5 R}\right]\right\} \qquad (25)$$

where R is the separation of the electron from the near nucleus.

In like manner we obtain:

$$(\sigma_g 2s | H' | \sigma_g 2p) = \frac{4}{3\sqrt{3}}\delta^5\left\{-e^{-2\delta R}\left[\frac{3R^2}{(2\delta)^2}+\frac{18R}{(2\delta)^3}+\frac{60}{(2\delta)^4}\right.\right.$$

$$\left.\left.+\frac{120}{(2\delta)^5 R}+\frac{120}{(2\delta)^6 R^2}\right]+\frac{120}{(2\delta)^6 R^2}\right\} \qquad (26)$$

$$(\sigma_g 2p | H' | \sigma_g 2p) = \frac{8}{15}\delta^5\left\{-e^{-2\delta R}\left[\frac{15R^2}{2(2\delta)^2}+\frac{90R}{2(2\delta)^3}+\frac{165}{(2\delta)^4}\right.\right.$$

$$\left.\left.+\frac{420}{(2\delta)^5 R}+\frac{720}{(2\delta)^6 R^2}+\frac{720}{(2\delta)^7 R^3}\right]+\frac{720}{(2\delta)^7 R^3}\right\} \qquad (27)$$

The matrix elements of $\cos\vartheta$ have been obtained by us previously for oxygen.[4] Hence all information is now available for the evaluation of the a_i in Eq. (21b) and hence the distorted orbitals. In Figure 1 we indicate the a_i of interest as a function of electron separation from the nearer nucleus. The perturbation scheme appealed to in distortion coefficient calculation may be expected to break down at some minimum proton separation.

We are now in a position to evaluate the U_{nn} of Eq. (15) for the ground electronic state of the oxygen molecule. We now make use of the appropriate distorted orbitals in Eq. (17) to obtain:

$$U_{nn} = V^{(0)} + 2a\left\{\left[.86842\, a_{2\sigma_g} + .13084\, a_{3\sigma_g} + .88962\, a_{2\sigma_u}\right] V_{2s}^{(0)}\right.$$

$$\left.+\left[.13076\, a_{2\sigma_g} + .86923\, a_{3\sigma_g} + .11040\, a_{2\sigma_u}\right] V_{2p}^{(0)}\right\} \qquad (28a)$$

$$V_{2s}^{(0)} = -(19.165R^2 + 9.184R + 4.465 + \frac{1}{R})e^{-5.718R} + \frac{1}{R} \tag{28b}$$

$$V_{2p}^{(0)} = -(3.523R^2 + 4.816R + 3.292 + \frac{1}{R})e^{-4.389} + \frac{1}{R} \tag{28c}$$

$$V^{(0)} = -(15.322 + \frac{3}{R})e^{-15.322R} - (38.330R^2 + 18.368R + 8.930 + \frac{2}{R})e^{-5.718R} - (14.092R^2 + 19.269R + 13.168 + \frac{4}{R})e^{-4.389R} \tag{28d}$$

In Eq. (28a) "a" is one-half the internuclear separation in the molecule.

We next evaluate Eq. (28a) numerically, the result being displayed as Figure II. We are able to make a reasonable fit to this figure with the much simplified function:

$$U_{nn} = e^{-.1209R}\left(\frac{3.14012}{R^2} - \frac{.46219}{R} + .030832\right) \tag{28e}$$

We now recall that our objective is the evaluation of Eq. (16) for some pair of electronic states and that U_{nm} not U_{nn} is needed for this evaluation, although the latter will be utilized in Eqs. (45). We now discuss our reason for the U_{nn} evaluation at this point.

The development leading to Eq. (29) illustrates our method of including polarization, a phenomena which is generally of some importance. The effects of polarization cannot be included in our derivation of U_{nm} where n and m correspond to the Schumann-Runge system. However, these effects likewise cannot be included in the corresponding contribution to U_{nn} above

or to the U_{nn} of another problem we discuss below. Even so these latter results are in reasonable agreement with experiment. The inference then is that our U_{nm} is nevertheless reasonably good. We now discuss this in more detail.

We have computed the interaction potential between two aligned oxygen molecules whose charge clouds are undistorted. The result is

$$V = -108.3 r^2 e^{-5r}$$

Vanderslice, Mason and Maisch[13] on the other hand have obtained the following from experiment:

$$V = 812 e^{-3.565r}$$

When we polarize certain molecular orbitals we compute the following potential:

$$V = 321 e^{-3.26r}.$$

Since this is effectively doubled for the off-axis case it is apparent that the improvement through the introduction of polarization is a considerable one. Even so, only the sigma orbitals were polarized; it was not possible to polarize the pi orbitals.

The evaluation of the a_i of Eq. (21b) is carried out between two states which must, of course be of the same symmetry. What we shall call our basis set consists of eight orbitals, three of one sigma symmetry ($1\sigma_g, 2\sigma_g, 3\sigma_g$), three of the other ($1\sigma_u, 2\sigma_u, 3\sigma_u$) one of one pi symmetry ($1\pi_u$) and one of the other ($1\pi_g$). It is obvious then that we can compute no a_i for the pi while we can compute them for the sigma. Even so our results for O_2 - O_2 are as given above,

that is, they are in reasonable agreement with experiment. We shall take this as support for the unpolarized orbitals to be used in computing U_{nm}.

We suppose that the inelastic collision of the electron with the oxygen molecule leads to the excitation of the upper state of the Schumann-Runge system. Hence, we will deal with an upper $^3\Sigma_u^-$ state and a lower $^3\Sigma_g^-$ state. The basic difference is that what was a π_u^- orbital in the ground state is a π_g^- orbital in the upper state. Our potential is then:

$$U_{nm} = \int \frac{\Psi(^3\Sigma_u^-)\Psi(^3\Sigma_g^-)}{r_{ie}} d\tau_i = \int \frac{/\pi_u\, /\pi_g}{r_{ie}} d\tau_i$$

The rather extreme reduction from Eq. (17) is due to the one particle nature of the interaction operator. This, coupled with the orbital orthogonality leads to the simple (and necessarily unpolarized) result. The entire molecular orbital (i.e., we do not reflect the contribution from the nether molecular atom) is here considered and only $r_>^{-1}$ is taken in the r_{ie}^{-1} expansion:

$$U_{nm} = (.7631)(.6619)\frac{\delta^5}{\pi}\left\{\int \frac{r_a^2 e^{-2\delta r_a}}{r_>} r_a^2 dr_a \int d\varphi \int \sin^3\vartheta_a\, d\vartheta_a - \int \frac{r_b^2 e^{-2\delta r_b}}{r_>} r_b^2 dr_b \right.$$

$$\left. \cdot \int d\varphi \int \sin^3\vartheta_b\, d\vartheta_b - \int \frac{r_a e^{-\delta r_a}}{r_>(\varphi,i)} r_b e^{-\delta r_b} \sin\vartheta_a \sin\vartheta_b\, d\tau + \int \frac{r_a e^{-\delta r_a}}{r_>(\varphi,i)} r_b e^{-\delta r_b} \sin\vartheta_a \sin\vartheta_b\, d\tau \right\}$$

$$= -C\left\{\left[\frac{R^2}{(2\delta)^2} + \frac{6R}{(2\delta)^3} + \frac{18}{(2\delta)^4} + \frac{24}{(2\delta)^5 R}\right] e^{-2\delta R} + \left[\frac{(R+a)^2}{(2\delta)^2} + \frac{6(R+a)}{(2\delta)^3}\right.\right.$$

$$\left.\left. + \frac{18}{(2\delta)^4} + \frac{24}{(2\delta)^5 (R+a)}\right] e^{-2\delta R} e^{-2\delta a} + \frac{24C}{(2\delta)^5 R} - \frac{24C}{(2\delta)^5 (R+a)}\right.$$

$$C = 82.0816$$

this may be plotted and fitted to:

$$U_{nm} = \frac{1.00861}{R} - \frac{1.00816}{R+a} \quad \begin{matrix} \delta = 2.275 \\ ) \; a = 2.282 \end{matrix} \tag{29}$$

Eq. (29) is now to be used in the evaluation of Eq. (16) with the result:

$$\sigma_{nm}(\vartheta) = \frac{k_n}{k_m} \frac{1}{4\pi^2} \left| \int \left[\exp\left\{ i(\underline{k}_n - \underline{k}_m) \cdot \underline{r}_j \right\} \right] \left\{ \frac{1.00861}{r_j} - \frac{1.00816}{r_j + a} \right\} d\tau \right|^2 \tag{30}$$

In the close-collision approximation we suppose that the electron follows a straight-line approach path until it collides head on with the molecule at which time it turns abruptly and proceeds out along its departure path. This approximation is not really very drastic for a close collision. If we now take angles as indicated in Figure III, the exponent in Eq. (30) becomes

$$k_n r_j \cos\delta - k_m r_j \cos\zeta = -k_n r_j \cos\epsilon - k_m r_j (\cos\vartheta \cos\epsilon - \sin\vartheta \sin\epsilon) \tag{31}$$

Thus the integral in Eq. (30) becomes

$$\iiint e^{i\left[k_m \sin\vartheta \sin\epsilon - (k_n + k_m \cos\vartheta)\cos\epsilon\right] r_j} \left(\frac{1.00861}{r_j} - \frac{1.00816}{r_j + a} \right) r_j^2 \sin\epsilon \, dr_j \, d\epsilon \, d\varphi \tag{32}$$

Certain obvious analytic integrations can be carried out in Eq. (32), but the lion's share would require numerical integration. It is not our purpose to accomplish this evaluation at this time.

Eqs. (30) and (32) yield the cross section for the excitation of the Schumann-Runge upper state through an electron collision along the molecular

symmetry axis. We now consider the ionization of the oxygen molecule by electron collision.

C. The Born Approximation for Electron Ionization

The only real difference in the Born cross section for ionization is, of course, in U_{nm}. The initial state of the molecule system is still the $^3\Sigma_g^-$ ground state while the final state is the free electron and the 0_2^+ ion in the state:

$$^2\Pi_g : \pi_g^+(\pi_u^-)^2(\pi_u^+)^2(\sigma_{3g})^2(\sigma_{2u})^2(\sigma_{2g})^2(\sigma_{1u})^2(\sigma_{1g})^2 \qquad (33)$$

The U_{nm} is here the integral over U of the product of the $1\pi_g^-$ orbital and the ejected electron wave function. The problem then is first to determine the wave function for the ejected electron.

Bates et al[6] and others,[7] have shown that in the case of the oxygen atom, the hydrogenic cross section for photo-ionization serves quite well to describe the oxygen phenomenon. The important point is not the method of ionization but the fact that the hydrogenic free electron wave function serves reasonably well. We shall use it in our evaluation. The orbitals are thus

$$\chi(1\pi_g^-) = .7631\sqrt{\frac{\delta^5}{\pi}}\, re^{-\frac{1}{2}r}\sin\theta e^{i\varphi} \qquad (34a)$$

$$\chi(kl) = (-)^{l+1} \frac{2}{\sqrt{1-e^{2\pi n'}}} \prod_{s=1}^{l} \sqrt{s^2+n^2} \frac{1}{2\pi (2kr)^{l+1}} \int e^{-\rho\xi} (\xi+\tfrac{1}{2})^{-in'-l-1}$$

$$(\xi-\tfrac{1}{2})^{in'-l-1} d\xi \cdot P_l^{|m|}(\cos\vartheta) \,, \quad \rho = -2ikr \,, \quad n' = \frac{1}{k} \tag{34b}$$

As usual our operator may be represented by the Legendre expansion:

$$\frac{1}{r_{ij}} = \sum \frac{(k-|m|)!}{(k+|m|)!} \frac{r_<^k}{r_>^{k+1}} P_k^{|m|}(\cos\vartheta_i) P_k^{|m|}(\cos\vartheta_j) \exp\left[im(\varphi_i-\varphi_j)\right] \tag{35}$$

of which we shall only take the first term. This means that, in order for the angular integrations to be non-zero, we must take a p angular state for the free electron. The contribution to U_{nm} from this may be written down as follows:

$$\int \chi(l\pi_j) \left(\frac{1}{r_{ij}} - \frac{8}{R}\right) \chi(kp)\, d\tau = .7631 \frac{1}{216} \frac{2\sqrt{1+n'^2}}{\sqrt{1-e^{-2\pi n'}}} \frac{1}{2\pi} \frac{1}{4k^2} \sqrt{\frac{35^5}{8\pi^2}}$$

$$\cdot \int \sin^2\vartheta\, e^{-i\varphi} e^{i\varphi} d\Omega \int (\xi+\tfrac{1}{2})^{-in'-2} (\xi-\tfrac{1}{2})^{in'-2} d\xi$$

$$\int e^{2ikr\xi} \frac{r}{r^2} e^{-\delta r} \left(\frac{1}{r_>} - \frac{8}{R}\right) r^2 dr \tag{36}$$

We now integrate over "r":

$$\frac{1}{R} \int_0^R e^{-(\delta-2ik\xi)r} r\, dr + \int_R^\infty e^{-(\delta-2ik\xi)r} dr - \frac{8}{R} \int_0^\infty e^{-(\delta-2ik\xi)r} r\, dr$$

$$= \frac{e^{-(\delta-2ik\xi)R}}{R(\delta-2ik\xi)^2} - \frac{7}{R(\delta-2ik\xi)^2}$$

We next integrate over ξ. When we substitute the above the -integral becomes

$$-\frac{e^{-\delta R}}{R} \int e^{2ikR\xi} (\xi+\tfrac{1}{2})^{-in'-2} (\xi-\tfrac{1}{2})^{in'-2} (\delta-2ik\xi)^{-2} d\xi - \frac{7}{R} \int (\xi+\tfrac{1}{2})^{-in'-2} (\xi-\tfrac{1}{2})^{in'-2} (\delta-2ik\xi)^{-2} d\xi$$

We shall evaluate this by integrating around the closed path in the complex plane continuing its pole and extending the path to infinity. The pole is at $\xi = -\frac{1}{2}i\frac{\delta}{k} = -\frac{1}{2}i\delta n'$. The value of such an integral is equivalent to $2\pi i \mathcal{R}$ when R is the residue at the pole, here of order two. We recall

$$\mathcal{R} = \frac{df}{d\xi} \qquad f = e^{2ikR\xi}(\xi+\tfrac{1}{2})^{-in'-2}(\xi-\tfrac{1}{2})^{in'-2}$$

When we make use of the relation:

$$\left(\frac{i\delta n'-1}{i\delta n'+1}\right)^{in} = e^{-2n'\coth^{-1}\delta n'}$$

The derivative may be evaluated as:

$$\left.\frac{df}{d\xi}\right|_{\xi=-\frac{1}{2}i\delta n'} = -\frac{2^6\pi k}{(\delta^2 n'^2+1)^2}e^{-2n'\coth^{-1}\delta n'} - \frac{2^7\pi i(in'-2)}{R(\delta^2 n'^2+1)}e^{-2n'\coth^{-1}\delta n'}$$

and when this is substituted in Eq. (36) the result is:

$$U_{nm} = .763\frac{\sqrt{\delta^5}2^4}{3k}\frac{e^{-2n'\coth^{-1}\delta n'}}{(\delta^2 n'^2+1)^2} - .763\frac{\sqrt{\delta^5}2^5}{3k^2}i\frac{(in'-2)}{(\delta^2 n'^2+1)^3}e^{-2n'\coth^{-1}\delta n'} \qquad (37)$$

We carry this no further but simply remark that one gets an equation similar to Eq. (32) and requiring numerical integration.

This ends our consideration of electron scattering for the present. We remark that we have failed to consider (1) elastic scattering, (2) dissociation and (3) the existence of rotational and vibrational motion. Under the Born approximation in use here, these pose no problems which are essentially different from those treated above and can be dealt with in this

general fashion at a later stage. However, it does appear that the excitation of electronic upper states and the ionization of the molecule are phenomena to be treated first in our scattering consideration.

There is a portion of the electronic excitation scattering which we have deliberately ignored and which certainly can be of definite importance. In the above sections we have considered what is generally referred to as the direct scattering. Now let us consider Eq. (16). We remark that in the exponential "r_j" is associated both with the incoming momentum vector and the outgoing momentum vector. This in essence describes the direct scattering. To this must be added a consideration of the exchange scattering, and, if we again refer to Eq. (16), our inbound electron will be associated only with the incoming momentum vector while some one of the molecular electrons will be associated with the outgoing momentum vector. This develops naturally from the fact that an exchange is made in the course of the collision. The treatment of this is certainly of some importance and must be presumed to be carried out in conjunction with and subsequent to the treatment of direct scattering.

SECTION III

PROTON SCATTERING BY DIATOMICS

A. Distorted Wave Treatment of Proton - Oxygen Scattering

This scattering problem cannot be treated by the Born approximation, for the velocity of a 50 KeV proton is a great deal less than that of the outer orbitals in the scattering molecules. Hence, we shall first appeal to what might be called a distorted wave approximation. * For the wave function for our molecule-proton system, we refer to Eq. (7) with the exchange effects dropped therefrom:

$$\Psi = \sum_n \Phi_{An}(\underline{r}_i)\,\psi_n(\underline{r}) \tag{38}$$

where now $\underline{r}$ is the inter-particle coordinate. Eq. (9) becomes

$$\left[\nabla_p^2 + k_n^2 - 2\left(\frac{Z_a}{r_{ap}} + \frac{Z_b}{r_{bp}} - \sum \frac{1}{r_{ip}}\right)\right] \sum \Phi_{An}(\underline{r}_i)\,\psi_n(\underline{r}) = 0 \tag{39}$$

We now multiply through on the left by $\Phi_{An}(\underline{r}_i)$ and integrate over the space of the molecular electrons. The result is:

$$\left\{\nabla_p^2 + k_n^2 - U_{nn}\right\}\psi_{np}(j) = \sum_{m \neq n} U_{nm}\,\psi_{mp}(j) \tag{40}$$

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* In general, the following derivation is the standard one, and the reader is referred to the textual references.

This is the familiar infinite set of coupled equations. We propose to simplify the equation by eliminating those U_{nm} which are of little consequence in the oxygen case.

We begin by eliminating spin flip U_{nm}. Since the Hamiltonian is linear in spin and Coulomb parts, two collisions are necessary for changes in both. Further the proton spin-electron spin interaction may well be small due to the mass relations in S. S. Therefore we need consider only triplet states. Further the symmetry of the integral must be the same as that involved in the dipole selection rules since the operator symmetry will be the same. These considerations eliminate a number of levels and, if we consider the first ten or so known levels, we find combination only with the upper state of the Schumann-Runge system. This is, of course, the level we considered for the electron scattering case.

We shall also include the continuum. Eq. (40) now becomes:

$$\{\nabla^2 + k_1^2 - U_1\}\psi_{1p} = U_{12}\psi_{2p} + \int U_{1c}\,dk\cdot\psi_{cp} \tag{41a}$$

$$\{\nabla^2 + k_2^2 - U_n\}\psi_{2p} = U_{21}\psi_{1p} + \int U_{2c}\,dk\cdot\psi_{cp} \tag{41b}$$

$$\{\nabla^2 + k_c^2 - U_c\}\psi_{cp} = \int U_{c1}\,dk\cdot\psi_{1p} + \int U_{c2}\,dk\cdot\psi_{2p} \tag{41c}$$

We shall treat these equations in cylindrical coordinates for which

$$\nabla^2 = \frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2} \tag{42}$$

We now consider the reduction of the wave functions to partial waves. As, for example, Geltman[8] has shown, one may choose a form for ψ on the basis that, in:

$$[\nabla^2 + k^2 - V]\psi = 0$$

as $V \to 0, \psi \to e^{i\underline{k}\cdot\underline{r}}$, a plane wave. We therefore choose the following form for:

$$\psi_1 = e^{i\underline{k}\cdot\underline{r}} + \chi_1 \tag{43a}$$

$$\psi_2 = \chi_2 \tag{43b}$$

$$\psi_3 = \chi_3 \tag{43c}$$

$$\chi_i = \sum_{\lambda=-\infty}^{+\infty} i^\lambda e^{-i\lambda\beta} F_{\lambda i}(\rho, z) e^{i\lambda\varphi} \tag{43d}$$

$$e^{i\underline{k}\cdot\underline{r}} = e^{ikz\cos\alpha} \sum i^\lambda e^{-i\lambda\beta} J_\lambda(k\rho\sin\alpha) e^{i\lambda\varphi} \tag{43e}$$

wherein α is the angle between $\underline{k}$ and the molecular symmetry axis and β is the azimuthal angle of $\underline{k}$.

The number of protons in the scattered wave crossing an element of area dS per second is:

$$v|\chi_i|^2 dS = v|\chi_i|^2 r^2 d\Omega$$

from which we can get our cross section as

$$\sigma = r^2|\chi_i|^2 \tag{44}$$

We now introduce an approximation which leaves a great deal to be desired but with which we do so little that it is of little moment anyway. We suppose the wave function

independent of the $\vec{z}$ -coordinate. Eqs. (43d) and (42) are substituted into Fqs. (41) with the result:

$$\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + k_1^2 - \left(\frac{\Lambda^2}{\rho^2}+U_{11}\right)\right\}F_{\lambda 1} = U_{12}F_{\lambda 2} + \int U_{1c}\,dk\cdot F_{\lambda c} \qquad (45a)$$

$$\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + k_2^2 - \left(\frac{\Lambda^2}{\rho^2}+U_{22}\right)\right\}F_{\lambda 2} = U_{21}F_{\lambda 1} + \int U_{2c}\,dk\cdot F_{\lambda c} \qquad (45b)$$

$$\left\{\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + k_c^2 - \left(\frac{\Lambda^2}{\rho^2}+U_{cc}\right)\right\}F_{\lambda c} = \int U_{1c}\,dk\cdot F_{\lambda 1} + \int U_{2c}\,dk\cdot F_{\lambda 2} \qquad (45c)$$

These wave functions will in each case have an asymptotic form corresponding to a cylindrical wave. An iterative method of solution is contemplated. The U_{11} and U_{22} will be given by Eq. (28e), the U_{12} by Eq. (29) and the U_{1c} by Fq. (37).

B. The Two State Impact Parameter Treatment

The central assumption in the impact parameter treatment is that of the classical path. The establishment of the validity of the classical path essentially assures us that we may deal with the projectile-target separation as a classical parameter. This validity is assured if the diffusion of the quantal wave packet representing the proton is such that during proton passage through the interaction region a separation is definable. In the present case, the applicability of the classical path is indeed assured.

Let us begin by writing out the Hamiltonian for our proton-oxygen system

$$H = \frac{Z^2}{r_{ab}} - \sum_{i=1}^{2Z}\left(\frac{1}{r_{ai}} + \frac{1}{r_{bi}}\right) + \sum_{i>j=1}^{2Z-1}\frac{1}{r_{ij}} + \frac{Z_a}{r_{ap}} + \frac{Z_b}{r_{bp}} - \sum_{i=1}^{2Z}\frac{1}{r_{pi}} \qquad (46)$$

where all symbols are the familiar standard ones and we shall work in atomic units.

We shall take ψ_i as the wave function for the initial proton-molecule system. By initial, we mean the system which existed at an infinite time in the past. In the same way ψ_f is the final wave function for our system. in this case the system which will exist at an infinite time in the future. The solution to the Schroedinger equation will assuredly be

$$\psi_i = \varphi_i(r_m)\frac{1}{r}\exp\left[-i\underline{k}\cdot\underline{r} - iE_r t\right] \qquad (47a)$$

$$\psi_f = \varphi_f(r_m)\frac{1}{r}\exp\left[i\underline{k}'\cdot\underline{r} - iE_r' t\right] \qquad (47b)$$

The φ_i refer to the molecular wave functions for oxygen. We shall continue to use the single determinant LCAO-MO form for the oxygen wave functions as computed by Kotani et al.[5] The k's in the equations correspond to the proton momentum before and after the collision. The 'r' is the radial coordinate of the proton with respect to the center of mass of the oxygen molecule; the energy indicated is the translational energy of the proton.

Eqs. (47) may be used to obtain the following approximate time-dependent system equation

$$\Psi(r,t) = a_i(t)\psi_i \exp(-iE_i t) + b_f(t)\psi_f \exp(-iE_f t) \qquad (48)$$

In this equation the a_i and b_i are the state growth coefficients corresponding to the initial and final state of the system. The complete determination of these coefficients constitutes the two state impact parameter treatment. The treatment of this problem to which we shall appeal was, for all practical purposes, introduced by Gurnee and Magee.[9] It has been discussed in connection with certain inelastic and charge transfer collisions by Bates[10] and somewhat improved upon by McCarroll.[11]

It is surely true that after an infinite time, the system will be in the final state. Therefore by the definition of the state growth coefficient the probability that the inelastic collision in question will have taken place is given by the square of this coefficient after such a time. Our objective in the calculation then is to determine this coefficient. When we substitute Eq. (48) into the Schroedinger equation, those terms present at infinite separation will cause a number of terms in the equation to drop out. The result is

$$a_i \exp(-iE_i t) H' \psi_i + b_f \exp(-iE_f t) H' \psi_f = i\dot{a}_i \psi_i \exp(-iE_i t) + i b_f \psi_f \exp(-iE_f t) \qquad (49)$$

wherein the H' has been taken as representing those terms in Eq. (46) relating to proton-molecule interaction.

We are now going to make the rather trivial transformation:

$$A_i = a_i \exp[-i\underline{k}\cdot\underline{r}]$$
$$B_i = b_i \exp[i\underline{k}'\cdot\underline{r}]$$

with the obvious effect on Fq. (49).

We multiply Eq. (49) through on the left first by $\varphi_i^*(\underline{r}_m)\exp[iE_i t]\,r\exp[iE_r t]$ and then by $\varphi_f^*(\underline{r}_m)\exp[iE_i t]\exp[iE'_r t]$ to obtain

$$a_i H'_{ii}\exp[-i\underline{k}\cdot\underline{r}] + b_f H'_{if}\exp[i\underline{k}'\cdot\underline{r}] = i\dot{a}_i\exp[-i\underline{k}\cdot\underline{r}] \qquad (50a)$$

$$a_i H'_{if}\exp[-i\underline{k}\cdot\underline{r}] + b_f H'_{ff}\exp[i\underline{k}'\cdot\underline{r}] = i\dot{b}_f\exp[i\underline{k}'\cdot\underline{r}] \qquad (50b)$$

where we define the matrix elements in Eqs. (50) as follows:

$$H'_{ii} = \int\varphi_i^* H'\varphi_i\,d\tau \qquad H'_{jj} = \int\varphi_j^* H'\varphi_j\,d\tau$$

$$H'_{ij} = H'_{ji} = \int\varphi_i^* H'\varphi_j\,d\tau \qquad (51)$$

Eqs. (50) may surely be added with the obvious result

$$i\dot{a}_i + i\dot{b}_f = (a_i + b_f)(H'_{ii} + H'_{if}) \qquad (52)\ *$$

We now introduce the specifics of the impact parameter treatment. Let us consider Figure IV. The proton in colliding with the molecule,

*Here $H'_{ii} = H'_{ff}$ leads to this result for, say, oxygen.

follows a straight-line path whose minimum separation is the impact parameter ρ. This straight-line path, for our purposes of consideration here lies entirely in the plane which is perpendicular to the molecular symmetry axis and which contains the molecular center of symmetry. Under these classical path conditions the time may be simply and linearly related to the distance along the path through the velocity. When we make this approximation Eq. (52) leads to

$$v \frac{d(A_i + B_f)}{dx} = -i(H'_{ii} + H'_{if}) \tag{53}$$

which the reader will immediately see to be equivalent to:

$$\int_{1}^{(A_i+B_f)} d[\ln(A_i+B_f)] = -i\int_{-\infty}^{x} \frac{1}{v}[H'_{ii} + H'_{if}]dx \tag{54}$$

of solution:

$$A_i + B_f = e^{-iQ} \qquad Q = \int_{-\infty}^{x} \frac{1}{v}(H'_{ii} + H'_{if})dx \tag{55}$$

The normality requirement on the wave function of Eq. (48) will lead to the following relationship between the state growth coefficients:

$$(\underline{\Psi}^*\underline{\Psi}) = a_i^* a_i + b_f^* b_f = 1 \tag{56}$$

The two state growth coefficients will at most be complex quantities so that under any condition we can replace them as follows:

$$A_i = \rho e^{i\omega} e^{-i\underline{k}\cdot\underline{r}} \qquad B_f = \rho' e^{i\omega'} e^{i\underline{k}'\cdot\underline{r}} \tag{57}$$

From Eqs. (56) and (57) we obtain the following relationship between the amplitudes of the two state growth coefficients

$$\rho^2 + |\rho'|^2 = 1 \tag{58}$$

which leaves the phase relationship to be determined. Eq. (57) as modified by Eq. (58) may now be substituted in Eqs. (50) and we obtain the following:

$$\rho e^{i\omega} H'_{ii} + \sqrt{1-\rho^2}\, e^{i\omega'} H'_{if}\, e^{i[(\underline{k}+\underline{k}')\cdot\underline{r}]} = -\dot{\omega}\rho e^{i\omega} + i\dot{\rho} e^{i\omega} \tag{59a}$$

$$\rho e^{i\omega} H'_{if}\, e^{-i(\underline{k}+\underline{k}')\cdot\underline{r}} + \sqrt{1-\rho^2}\, e^{i\omega'} H'_{ff} = -\dot{\omega}'\sqrt{1-\rho^2}\, e^{i\omega'} + i\dot{\sqrt{1-\rho^2}}\, e^{i\omega'} \tag{59b}$$

Eqs. (59) provide us with four equations, two real and two imaginary. The imaginary equation arising from Eq. (59) allows us but two choices

$$i\dot{\rho} e^{i\omega} = 0 \quad \text{or} \quad b_+ = i\sqrt{1-\rho^2}\, e^{i\omega}$$

The solution requiring the time derivative of the initial state amplitude to be zero would mean that no transition could be induced by the collision. This forces our acceptance of the second equation which yields the final state growth coefficient. Our state growth coefficients are now:

$$a_i = \rho e^{i\omega} \qquad b_f = i\sqrt{1-\rho^2}\, e^{i\omega} \tag{60}$$

We consider the imaginary equation from Eq. (59) as modified by

Eq. (60):

$$\dot{\rho} = \sqrt{1-\rho^2}\, H'_{if}\, e^{i[(\underline{k}+\underline{k}')\cdot\underline{r}]}$$

Again appealing to the classical path relationship between distance and time, we may obtain the following equation from this:

$$\int_{\rho_i}^{\rho_f} \frac{d\rho}{\sqrt{1-\rho^2}} = \int_{-\infty}^{x} \frac{1}{v} H'_{if}\, e^{i[(\underline{k}+\underline{k}')\cdot\underline{r}]}\, dx \tag{61}$$

From this equation one may obtain the following expression for the final state growth coefficient:

$$|b_f(\infty)|^2 = |\sqrt{1-\rho_\infty^2}|^2 = |\sin\left[\int_{-\infty}^{+\infty} \frac{1}{v} H'_{if}\, e^{i[(\underline{k}+\underline{k}')\cdot\underline{r}]}\, dx\right]|^2 \tag{62}$$

The probability for transition and hence for the inelastic scattering under consideration here is the square of this state growth coefficient after infinite time. In order to obtain the cross section, we simply average over impact parameter with the following results:

$$\sigma = 2\pi \int_0^\infty |b_f(\infty)|^2 \rho\, d\rho \tag{63}$$

The expansion of the sine leads to an expression whose first term Arthurs[12] has shown is equivalent to the Born approximation.

C. The Two State IP Treatment of the Proton Oxygen Case

We write down the interaction Hamiltonian as follows:

$$H' = \frac{8}{r_a} + \frac{8}{r_b} - \sum_{i=1}^{16} \frac{1}{r_i} \tag{64}$$

Our first task is the evaluation of this Hamiltonian over the two molecular states involved in the inelastic collision. This matrix element was defined by our development, and we recall that it involves only the molecular coordinates. A point here is that we should evaluate this matrix element over the states of the molecule as perturbed by the incident proton, but we refer to our discussion in connection with Eq. (28e).

This matrix element is given by Eq. (29) with opposite sign:

$$H'_{if} = -\frac{1.00861}{R} + \frac{1.00816}{R+a} \tag{65}$$

Eq. (65) describes that case where the proton proceeds in along the molecular figure axis. We shall suppose one-third of the oxygen molecules are so aligned, that is, we shall suppose their internuclear axis are aligned along, say, the z-axis which is taken as the proton path. The other two-thirds of the molecules are aligned one-half along the x-axis and one-half along the y-axis. Let us consider this other two-thirds.

Let us suppose the proton is inbound toward the oxygen molecule in the plane which is perpendicular to the molecular symmetry axis and which contains the molecular center of symmetry. The π orbital is identically zero in this plane with the result that U_{nm} is identically zero. As we move the proton path away from this plane it is apparent that U_{nm} will increase to a maximum at the internuclear axis. But it is also apparent that the majority of collisions will occur more nearly under this

than under the former (perpendicular central plane). Therefore we are simply going to assume the axis collision path to be valid.

Eq. (65) is now substituted into Eq. (63). We suppose that the proton maintains its initial velocity -- which corresponds to the momentum k -- until it reaches a particular point on the trajectory. At this point it instantaneously attains its final velocity -- which corresponds to the momentum k'. The space point selected for the change is x = 0. The inner product in the exponential now becomes:

$$\underline{k}\cdot\underline{r} = -kr\cos(\pi-\vartheta) = kr\left(\frac{x}{r}\right) \tag{66}$$

and the bracketed expression in Eq. (63) becomes

$$\frac{1}{v}\int_{-\infty}^{0} H'_{if}\exp[i(k-k')x]\,dx + \frac{1}{v'}\int_{0}^{\infty} H'_{if}\exp[-i(k-k')x]\,dx \tag{67}$$

Eq. (67) may be re-written as:

$$\left(\frac{1}{v}+\frac{1}{v'}\right)\int_{0}^{\infty} H'_{if}\cos[(k-k')x]\,dx + i\left(\frac{1}{v}-\frac{1}{v'}\right)\int_{0}^{\infty} H'_{if}\sin[(k-k')x]\,dx \tag{68}$$

The right side of Eq. (63) now becomes:

$$\sin^2\left\{\left(\frac{1}{v}+\frac{1}{v'}\right)\int_{0}^{\infty} H'_{if}\cos[(k-k')x]\,dx\right\}$$

$$+\sin^2\left\{\left(\frac{1}{v}-\frac{1}{v'}\right)\int_{0}^{\infty} H'_{if}\sin[(k-k')x]\,dx\right\} \tag{69}$$

The second term in Fq. (69) becomes important at energies below one thousand electron volts. At one KeV for our case it is about two orders

of magnitude smaller than the first term for all values of the impact parameter. We therefor drop the term.

For one thosand volts and above:

$$\cos[(k-k')x] \doteq 1$$

Thus Eq. (63) becomes:

$$|b_f|^2 = \sin^2\left[\left(\frac{1}{v} + \frac{1}{v'}\right)\int_0^\infty H'_{if}\,dx\right] \qquad (70)$$

which is what would have resulted from an assumption of post and prior momentum equality.

This expression was evaluated on a desk computer for a sufficient number of impact parameters to allow evaluation of Eq.(63) for the Schumann-Runge excitation and for values of the proton translational energy ranging from 1 to 50 KeV. A word on this latter evaluation is in order.

If one traces the behavior of $|b_f|^2$ inward from large ρ one finds that it is a monotonically increasing function until a point a few units from the nucleus is reached. At this point the function passed through a maximum and then oscillates more and more rapidly at lesser separations. The integration inward is numerical to the first minimum and will be discussed in a moment. From the first minimum, however, we take $|b_f|^2 \equiv \frac{1}{2}$ so that the integral has a value $\frac{1}{4}\rho_{min}$ for this inner portion.

If one retains the infinite upper limit for the integral in Eq.(63) the form of the interaction will lead to a divergence. This is a formal

difficulty at worst since the upper limit on the interaction will not be infinite; it will be determined by the shielding effect of the other particles. We choose the upper limit in Eq. (63) as the Debye radius. For the present, however, we may not specifically evaluate this since we are working with no particular temperature and density. We choose the limit as fifty units.

In Figure V we illustrate the behavior of the cross section for various energies as a function of impact parameter. The total cross sections which result are given for this energy range in Figure VI.

We show that Eq. (62) reduces to the Born approximation for large v or small H'_{if}. We first make the following approximation:

$$b_f = \sin\left\{ \int \frac{1}{v} H'_{if} \exp\left[i (\underline{k} + \underline{k}') \cdot \underline{r} \right] dx \right\}$$

$$\doteq \sin\left\{ \frac{1}{v} \int H'_{if} \exp\left[\frac{i}{v} (E_f - E_i) x \right] dx \right\}$$

which depends for its validity on large v. Next the sum is expanded in a MacLaurin series:

$$b_f = \frac{1}{v} \int H'_{if} \exp\left[\frac{i}{v} (E_f - E_i) x \right] dx$$

$$- \frac{1}{3! v} \left\{ \int H'_{if} \exp\left[\frac{i}{v} (E_f - E_i) x \right] dx \right\}^3 + \cdots$$

which reduces to its first term for large v or small H'_{if}. Arthurs[12] has shown that this term is equivalent to the Born approximation.

SECTION IV

THE MULTI STATE IMPACT PARAMETER TREATMENT

We consider the molecule as possessing a large number of bound states. In this development we do not include continuum states for the molecule. We take the following expression as the wave function for the proton-molecule system:

$$\Psi = \sum c_i(t)\varphi_i(\underline{r}_m)\frac{1}{r}\exp\left[-i\underline{k}_i\cdot\underline{r} - iE_{ti}t\right] \tag{71}$$

In this equation each term is an exact solution to the Schroedinger equation for infinite separation of the proton-molecule system. The subscript "i" runs over the states of the molecule. When Eq. (71) is substituted into the Schroedinger equation, all terms save the following drop out:

$$\sum c_i(t)\exp[-iE_it]H'\varphi_i(\underline{r}_m)\frac{1}{r}\exp\left[i\underline{k}'_m\cdot\underline{r} - iE'_{ti}t\right]$$

$$= i\sum \dot{c}_i(t)\exp[-iE_it]\varphi_i(\underline{r}_m)\frac{1}{r}\exp\left[i\underline{k}'_m\cdot\underline{r} - iE'_{ti}t\right] \tag{72}$$

We remark here that the k_i is negative for i = 1 and positive of various values for all other i. The normality condition for the wave function leads to

$$(\Psi^*,\Psi) = \sum c_i^* c_i = 1 \tag{73}$$

Again we take a general form for the state growth coefficient as follows:

$$c_i = \rho_i e^{i\omega_i} \tag{74}$$

At minus infinity of time we again suppose the coefficient corresponding to the molecular ground state to be unity. Depending on the transition in which we interest ourselves we then are concerned with the value of the upper state coefficient after an infinite time. This we proceed to determine.

First we make the following rather trivial transformation in Eq. (72):

$$C_i = c_i e^{i \underline{k}_i' \cdot \underline{r}} \tag{75}$$

We shall now multiply Eq. (72) through on the left, first by $\varphi_1^* r \exp[-i(E_1+E_{r1})t]$ then by $\varphi_2^* r \exp[-i(E_2+E_{r2})t]$ and so on. The result is:

$$\sum C_i H'_{1i} = i \dot{C}_1 \tag{76a}$$

$$\sum C_i H'_{2i} = i \dot{C}_2 \tag{76b}$$

$$\sum C_i H'_{3i} = i \dot{C}_3 \quad \text{etc.} \tag{76c}$$

We now add Eqs. (76) to obtain:

$$\sum_j \sum_i C_i H'_{ji} = i \sum_i \dot{C}_i \tag{77}$$

Eq. (77) may be rewritten as follows:

$$\sum_i \left[C_i \sum_j H'_{ji} - i \dot{C}_i \right] = 0 \tag{78}$$

There are two ways in which this equation could hold. First the various terms or certain of the various terms could be non-zero while some remain zero under all conditions. This is certainly not true at

minus infinity of time since there the time rate of change of the coefficient is zero while the matrix element of the perturbing Hamiltonian is zero. Hence it follows that Eq. (78) is zero because each term in Eq. (78) is zero. We now introduce the impact parameter treatment and again replace "t" by "x". Under these conditions any term in Eq. (78) may be written as

$$\frac{dC_i}{dx} = -\frac{i}{v}\sum_j H'_{ji} \cdot C_i \tag{79}$$

Eq. (79) has the familiar and immediate solution:

$$C_i = e^{-iQ_i} \qquad Q_i = -i\int_{-\infty}^{x}\frac{1}{v}\sum_j H'_{ji}\,dx \tag{80}$$

Relationships among the ρ_i and the ω_i are required now for the completion of the calculation. We begin by forming the column matrix which we term the amplitude matrix and which may be represented as:

$$\underline{a} = (\rho_i e^{-i\omega_i}) \tag{81}$$

With this definition the Schroedinger equation may be written in matrix form as follows:

$$\underline{H}\,\underline{a} = i\frac{d}{dt}\underline{a} \tag{82}$$

We multiply this equation through on the right by the associate matrix $\underline{a}^+$ to obtain:

$$\underline{H}\,\underline{a}\,\underline{a}^+ = i\left(\frac{d}{dt}\underline{a}\right)\underline{a}^+ \tag{83}$$

Let us write down the product of the matrix "a" and its associate as follows:

$$\underline{a}\,\underline{a}^{\dagger} = \underline{b} \tag{84}$$

This matrix is possessed of no inverse and its adjoint matrix is a null matrix. However, we may form the pluverse matrix which when it multiplies the matrix $\underline{b}$ on the right yields the null matrix. We prove this as follows.

First of all the elements of the pluverse matrix are defined as follows:

$$b_{ii}^{\natural} = \sum_{j \neq i} b_{jj} \tag{85a}$$

$$b_{ij}^{\natural} = - b_{ij} \tag{85b}$$

We now write out a typical element of the $\underline{b}\,\underline{b}^{\natural}$ product matrix as

$$\begin{aligned} b_{ij} &= a_{i1}\, a_{j1}^{\dagger} = \rho_i \rho_j \\ c_{ln} &= (\underline{b}\,\underline{b}^{\natural})_{ln} = \rho_l \rho_n \sum_{i \neq n}{}' \rho_i^2 - \sum_{i \neq n}{}' \rho_l \rho_i^2 \rho_n \\ &= \rho_l \rho_n \left[\sum{}' \rho_i^2 - \sum{}' \rho_i^2 \right] \equiv 0 \end{aligned} \tag{86}$$

which demonstrates that multiplication on the right by the pluverse matrix yields the null matrix.

We multiply Eq. (83) through on the right to obtain the following :

$$i \left(\frac{d}{dt} \underline{a} \right) \underline{a}^{\dagger} \underline{b}^{\natural} = \underline{0} \tag{87}$$

An an example we treat the two state case. First of all the coefficient matrix and the product of this matrix with its associate may be written down as:

$$\underline{a} = \begin{pmatrix} \rho_1 e^{-i\omega_1} \\ \rho_2 e^{-i\omega_2} \end{pmatrix} \quad \underline{b} = \underline{a}\,\underline{a}^{+} = \begin{pmatrix} \rho_1^2 & \rho_1\rho_2 \\ \rho_1\rho_2 & \rho_2^2 \end{pmatrix} \tag{88}$$

We may form $\underline{b}^{\gamma}$ through Eqs. (85) as

$$\underline{b}^{\gamma} = \begin{pmatrix} \rho_2^2 & -\rho_1\rho_2 \\ -\rho_1\rho_2 & \rho_1^2 \end{pmatrix} \tag{89}$$

The matrix manipulation indicated by Eq. (87) next leads to two equations in the amplitudes and phases. First through, the assumption of a constant difference between the two phases leads to the following expression:

$$e^{-i(\omega_1-\omega_2)} = a+ib = \sqrt{1-b^2}+ib \tag{90}$$

Eq. (90) now allows us to write down one of the two equations arising from Eq. (87) as:

$$\dot{\rho}_1\rho_1\rho_2^2\left[1-\sqrt{1-b^2}-ib\right]+i\dot{\omega}\rho_1^2\rho_2^2\left[-1+\sqrt{1-b^2}+ib\right]=0 \tag{91}$$

The solution is:

$$b=1 \tag{92}$$

The normality condition, of course, leads immediately to the relationship among the amplitudes and we have obtained the same result

which was obtained in the previous section in a somewhat more straightforward, if less generally applicable, manner.

SECTION V

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"Excitation and Ionization of Atoms by Electron Impact". H. S. W. Massey, Handbuch der Physik XXXVI, Page 307 (1956).

Professor Takayanagi has developed a very comprehensive explanatory bibliography of non-nuclear scattering phenomena. It consists of three parts plus a supplement which is dated August 1962. Although No. 1 is no longer available it is understood that the remaining parts may be obtained by writing

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The bibliography is broken down as follows:

Collision Theory. Part 1
I. Excitation and Ionization of Atoms by Electron Impact
II. The collision of Electrons with Molecules
III. Theory of Inelastic Molecular Collisions

Collision Theory. Part II
IV. Atom - Ion Atom - Atom Inelastic Collisions
V. Charge Transfer

Collision Theory. Part III
VI. Inelastic Collisions of Electrons with Atoms or Molecules (experimental)
VII. Photoionization and Radiative Recombination
VIII. Theory of Intermolecular Forces

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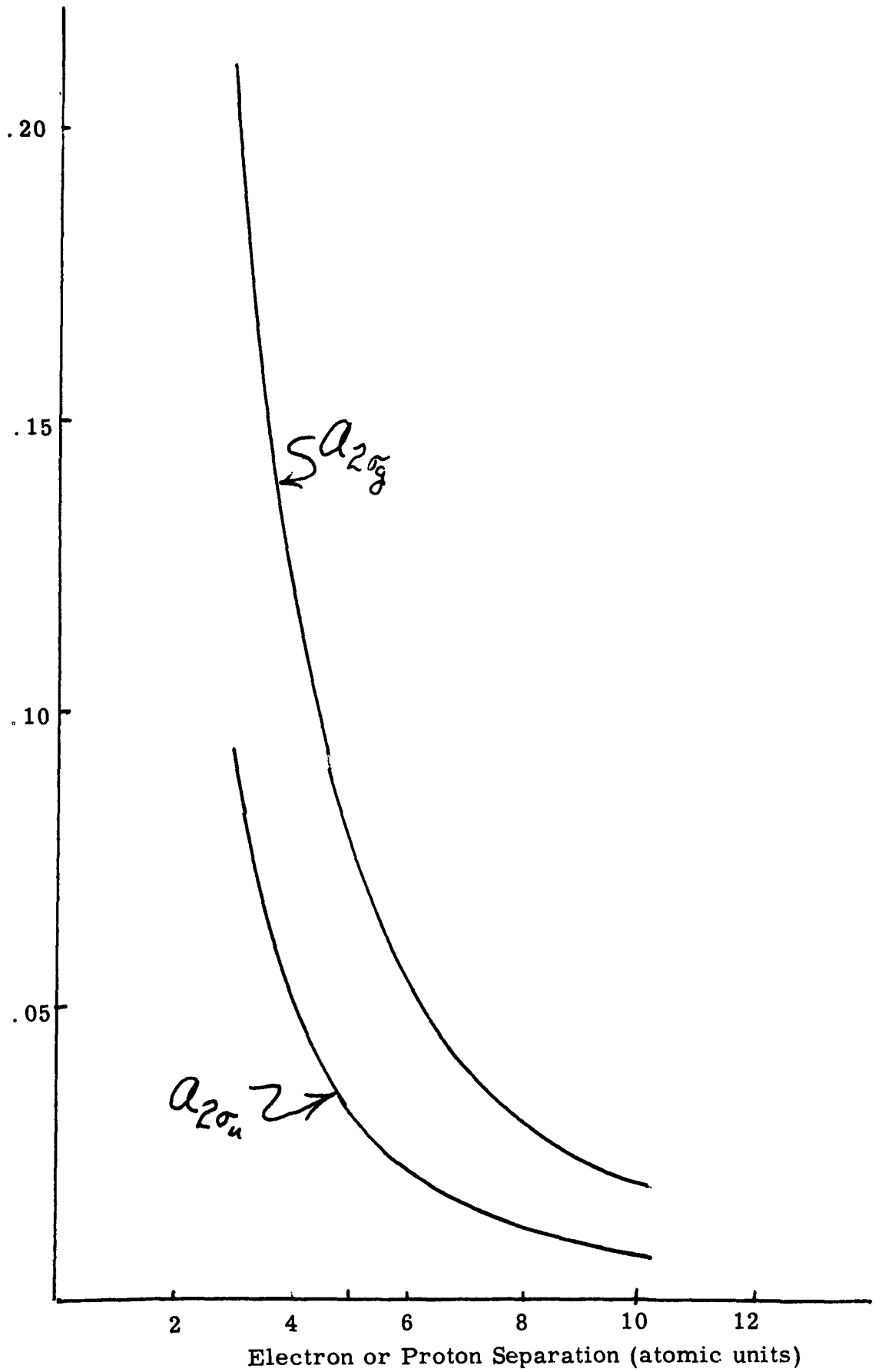

Figure I. The molecular distortion parameters for the electron-oxygen or proton-oxygen case.

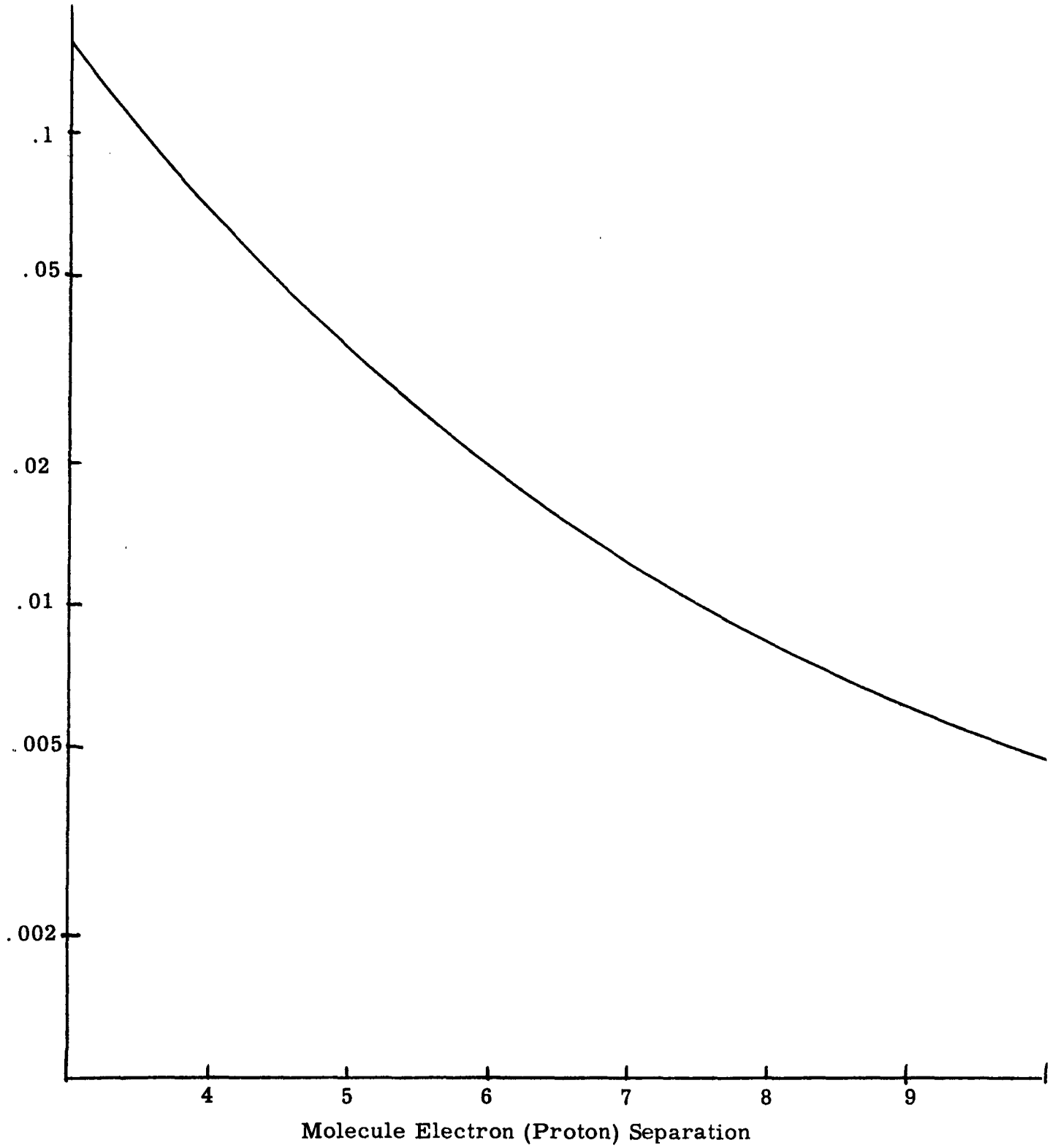

Figure II. The electron or proton oxygen interaction potential to include polarization.

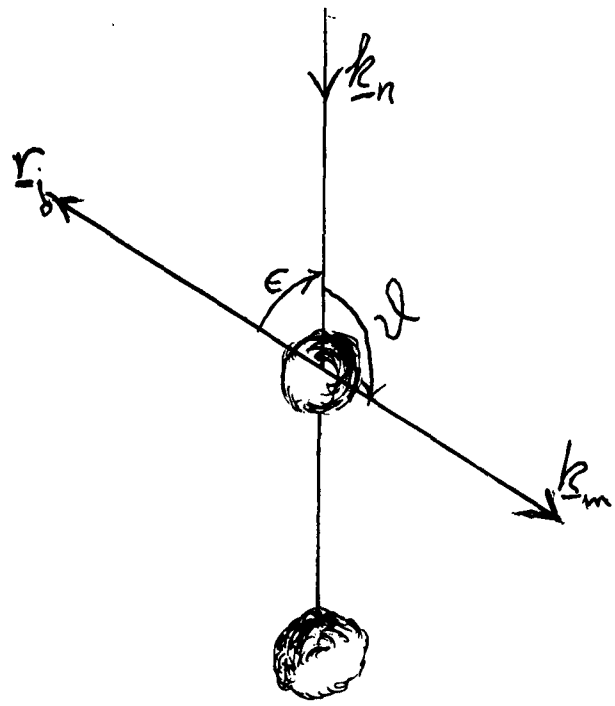

Figure III. The definition of the angles referred to in Eq. (30) and subsequent.

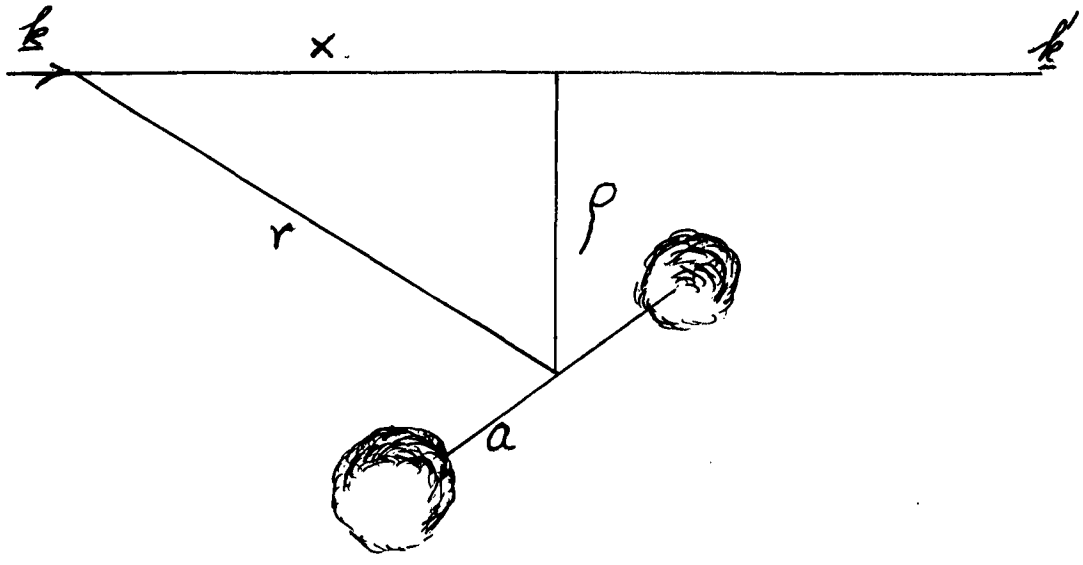

Figure IV. The geometry for the Impact Parameter treatment of the proton-oxygen collision.

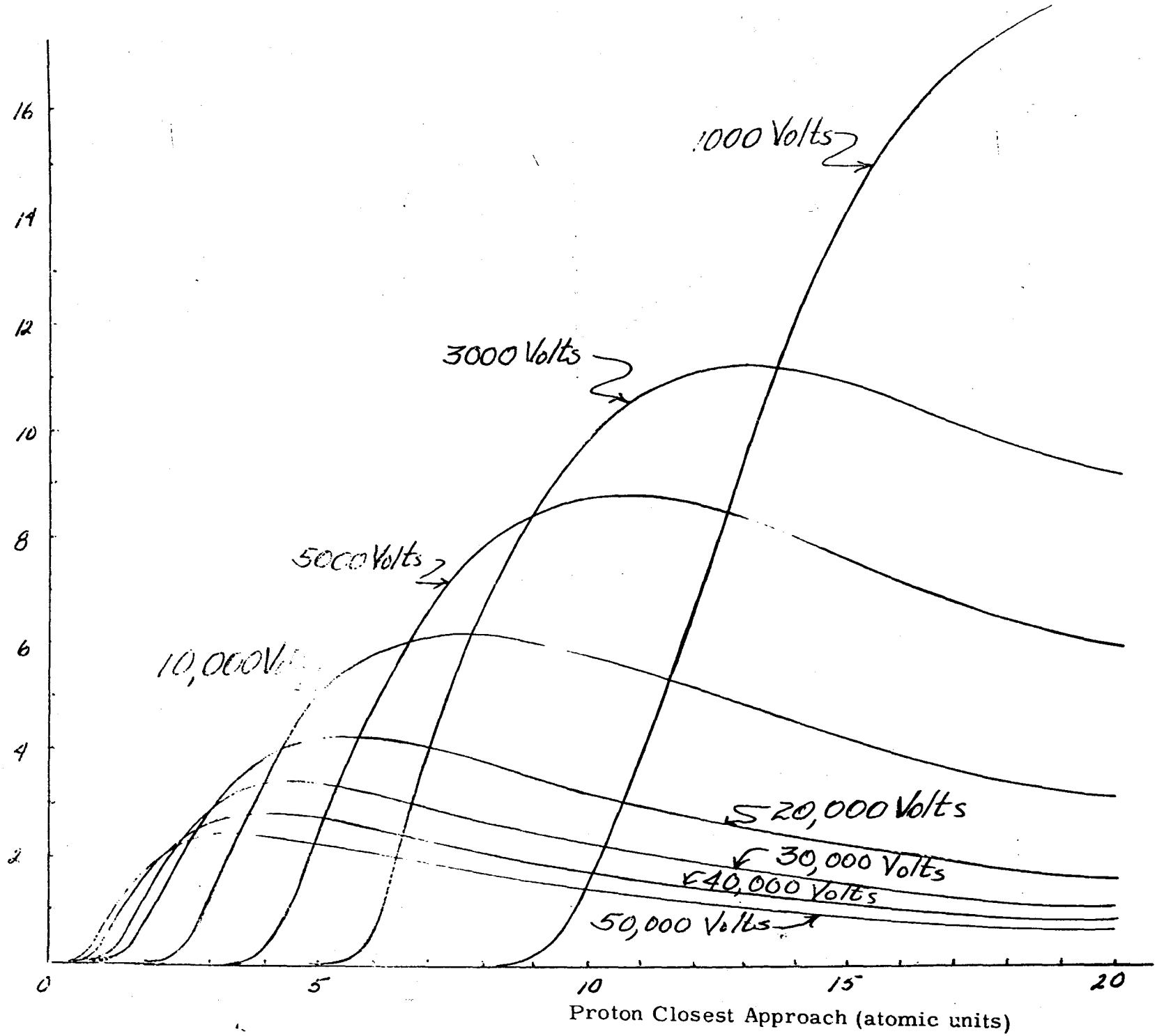

Figure V. The cross section integrand for various proton energies.

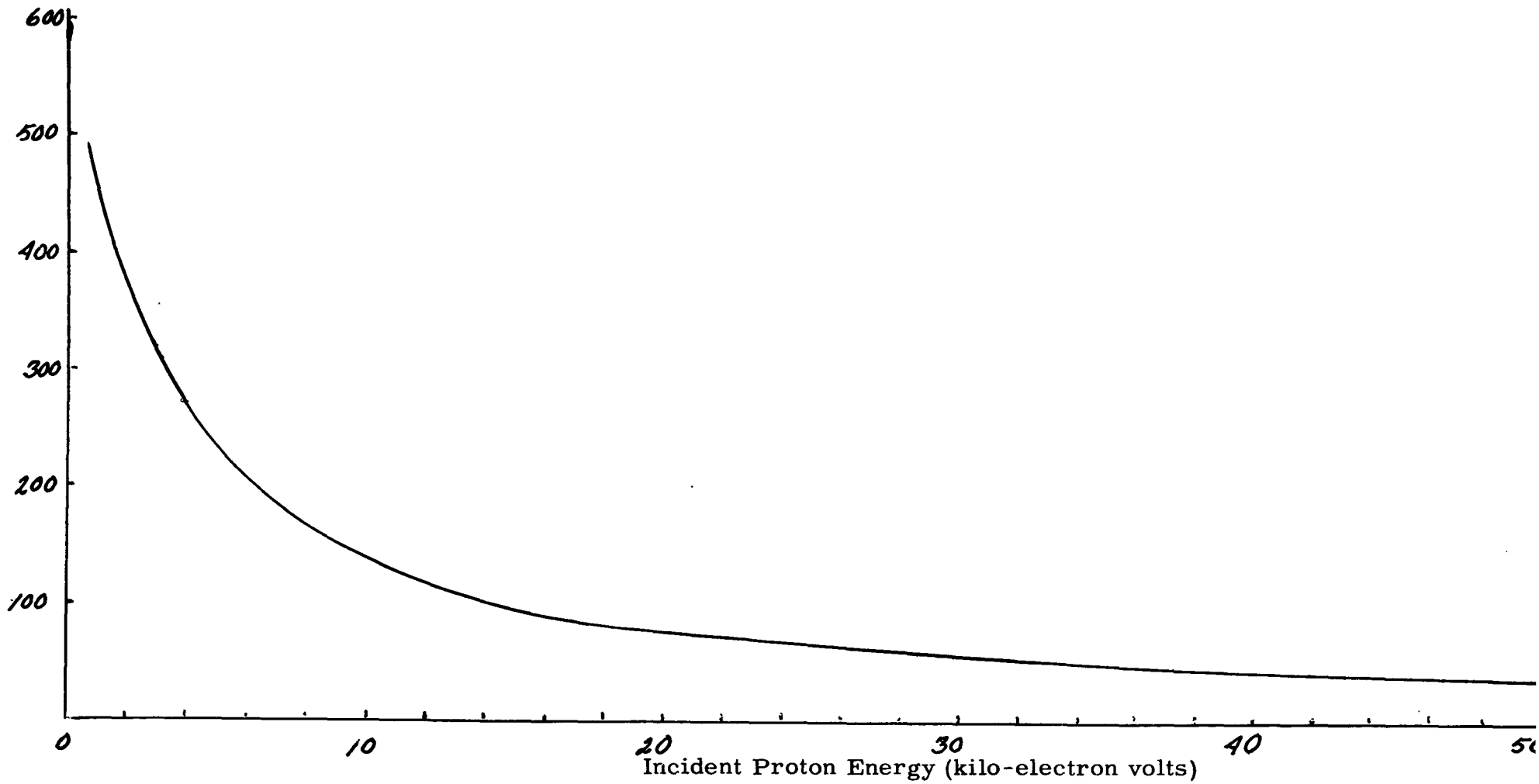

Figure VI. Total cross section for proton excitation of the Schumann-Runge system in units of $2\pi a_o^2$

Air Force Cambridge Research Laboratories, Bedford, Massachusetts. PROTON AND ELECTRON SCATTERING BY DIATOMIC MOLECULES by R. G. Breene, Jr., Physical Studies, Inc., Centerville, Ohio. April 1963. 86 pages. (Project 8658; Task 86580) Contract AF19(628)-476 (AFCRL-63-697). The scattering of electrons by diatomic molecules, specifically, oxygen, is first considered. The treatment is restricted in such a way that electronic computing machinery is not required for solution. The Born approximation is applicable, and the appropriate equations are developed but not solved. The proton-molecule problem is next treated for the inelastic scattering of one

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